Reynolds' Transport Theorem in a Discrete System

Edward Smith

Mechanical Engineering
Imperial College London

Outline

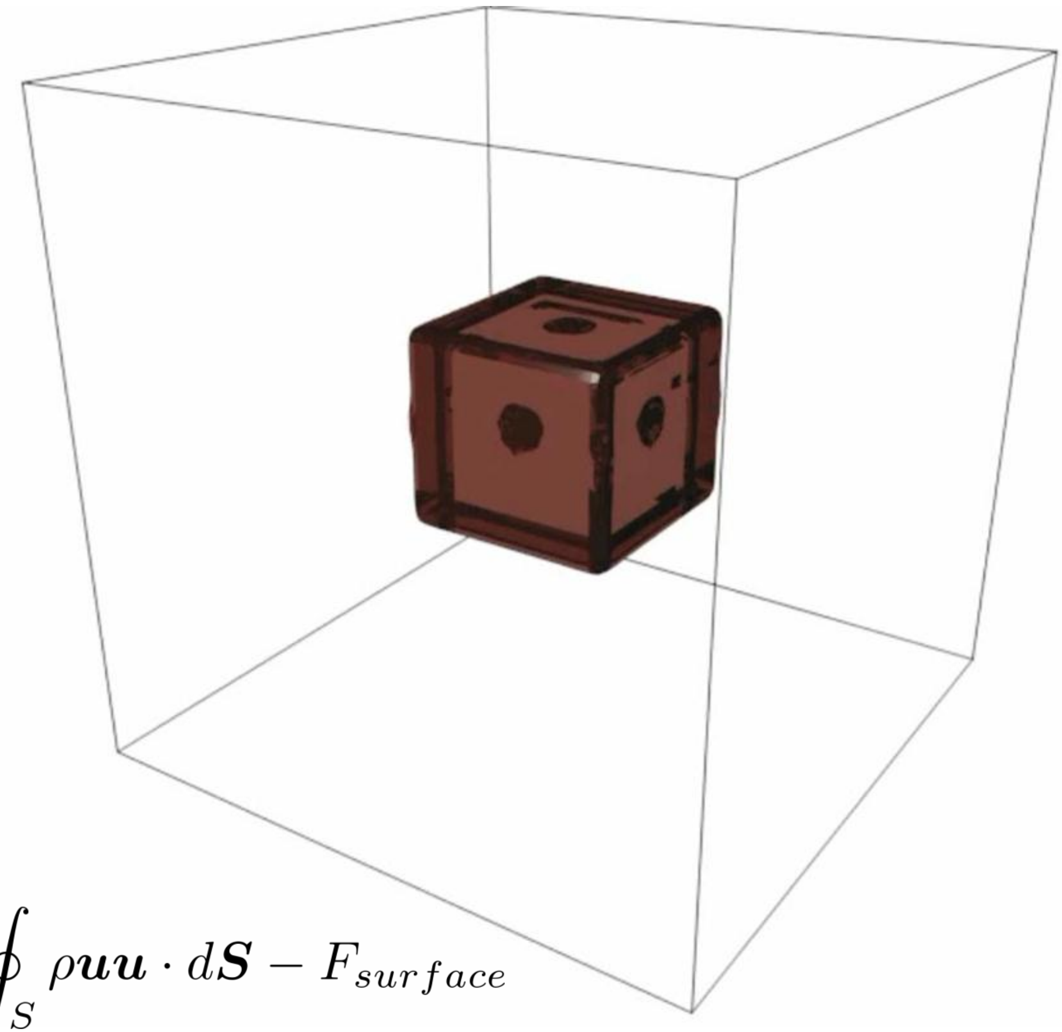
- **Introduction**
  - Reynolds' transport theorem
  - Discrete models (molecular dynamics)
  - Irving and Kirkwood (1950)
- **Discrete Form of Reynolds' Transport Theorem**
  - Control Volume Function
  - Reynolds' transport theorem using the control volume function
  - Application to microscopic pressure
- **Results**
  - Numerical simulations of Couette flow and shockwaves
  - Applying the method to coupling
  - Application to other discrete systems

Introduction

Reynolds' Transport Theorem

- **Conversion of a Lagrangian system to an Eulerian Control Volume**
  - Mass Conservation

$$\frac{d}{dt}\int_V \rho dV = 0$$
$$= \int_V \frac{d\rho}{dt} dV + \oint_S \rho \boldsymbol{u} \cdot d\boldsymbol{S}$$

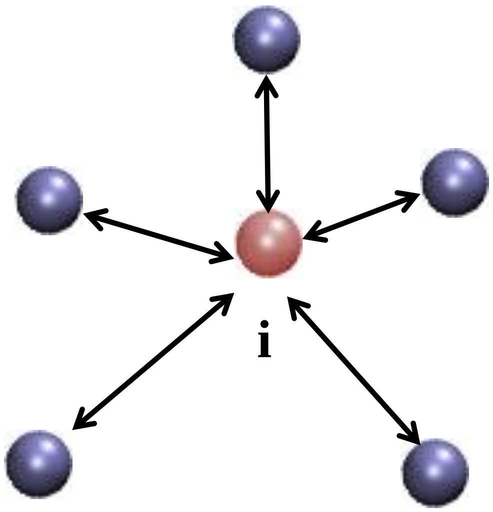


  - Momentum Balance

$$\frac{d}{dt}\int_V \rho \boldsymbol{u} dV - F_{surface} = 0$$
$$= \int_V \frac{d\rho \boldsymbol{u}}{dt} dV + \oint_S \rho \boldsymbol{u}\boldsymbol{u} \cdot d\boldsymbol{S} - F_{surface}$$

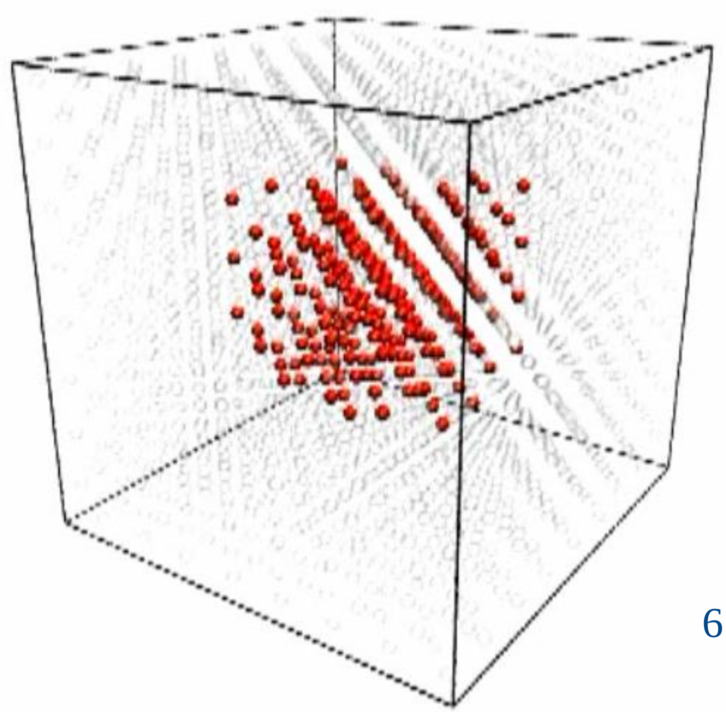
Discrete models (molecular dynamics)

- **Discrete Molecules in continuous space**
  - Governed by Newton's Law for an N-body system
  - Point particles with pairwise interactions only



$$m_i \ddot{\boldsymbol{r}}_i = \mathbf{F}_i = \sum_{i \neq j}^{N} \boldsymbol{f}_{ij} \qquad \begin{array}{l} \ddot{\boldsymbol{r}}_i \to \dot{\boldsymbol{r}}_i \\ \dot{\boldsymbol{r}}_i \to \boldsymbol{r}_i(t) \end{array}$$

- **Discrete N-body system defined in terms of sums**
  - Sum over entire system defines Lagrangian system
  - How do we get an Eulerian description?



$$\rho_{system} = \frac{1}{M} \sum_{i=1}^{M} m_i \qquad \int_V \rho(\boldsymbol{r}, t) dV = ?$$

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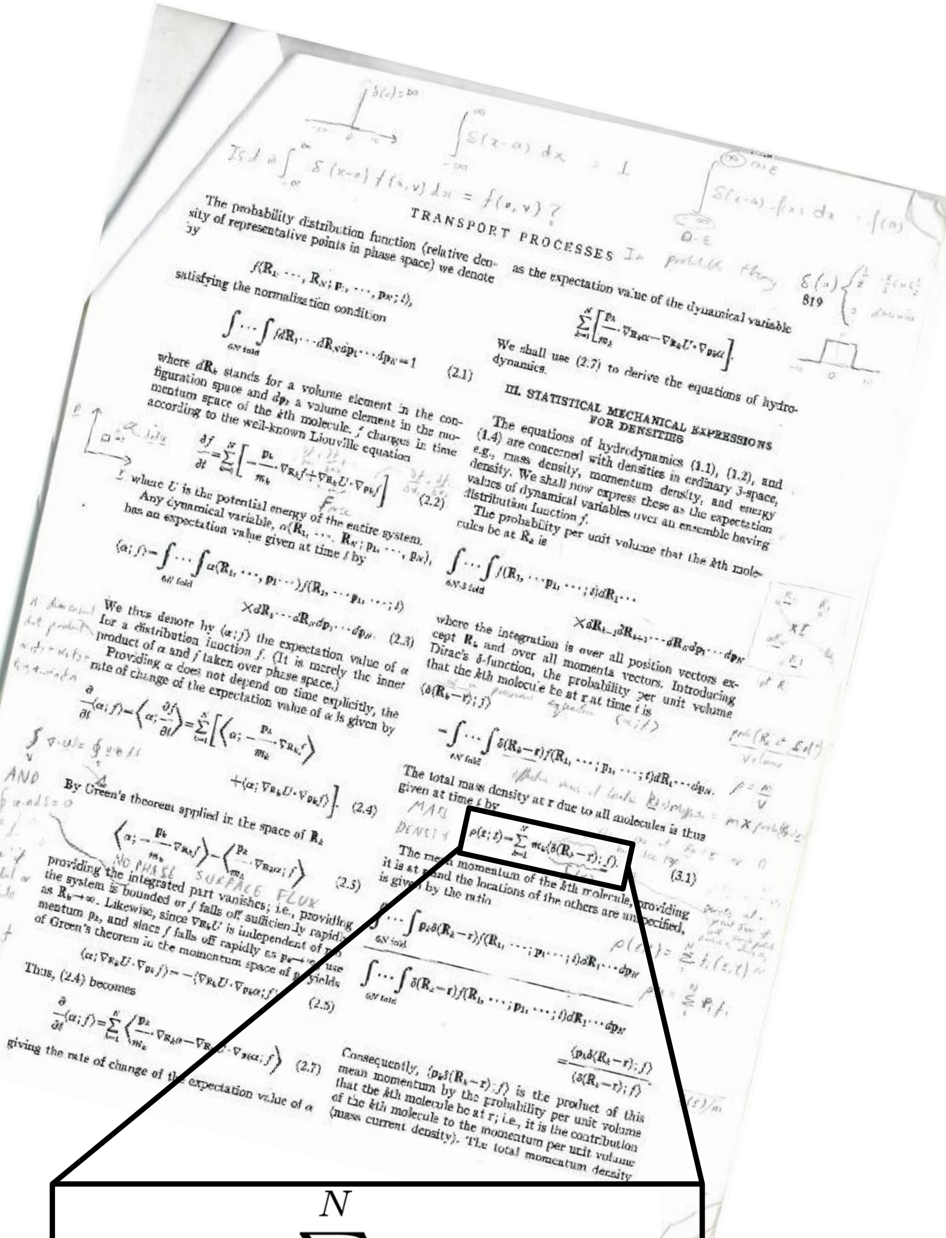
Irving and Kirkwood (1950)

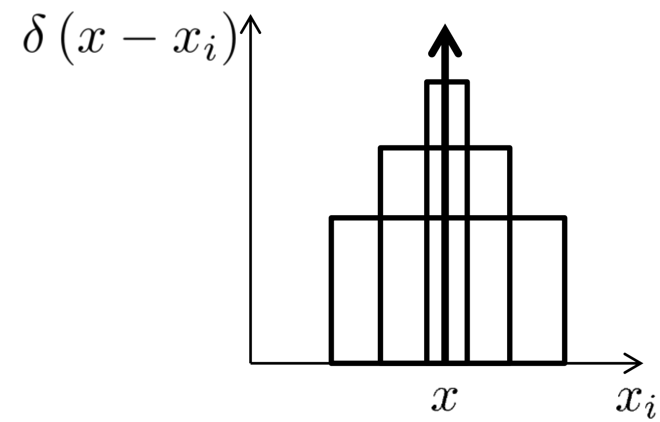


$$\rho(\boldsymbol{r},t)=\sum_{i=1}^{N} m_i\delta\left(\boldsymbol{r}-\boldsymbol{r}_i\right)$$

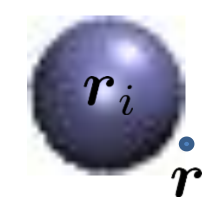
Selecting Functions

- **The Dirac delta selects molecules at a point**
  - Infinitely high, infinitely thin peak
  - Equivalent to the continuum differential formulation at a point

$$\rho(\boldsymbol{r}, t) = \sum_{i=1}^{N} m_i \delta\left(\boldsymbol{r} - \boldsymbol{r}_i\right)$$

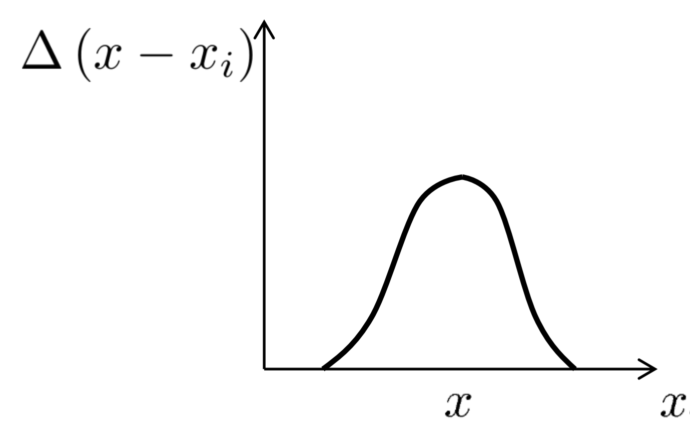


- **Cannot be applied directly in a molecular simulation as $\boldsymbol{r}_i$ is never exactly equal to $\boldsymbol{r}$**



- **Relaxed weighting function used by Hardy(1981), Hoover (2009), Murdoch (2010) and others**

$$\rho(\boldsymbol{r}, t) \neq \sum_{i=1}^{N} m_i \Delta\left(\boldsymbol{r} - \boldsymbol{r}_i\right)$$



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Discrete
Reynolds' Transport Theorem

More information

- **Further details of mathematics and numerical simulations are available in the recently published paper in Physical Review E**

PHYSICAL REVIEW E **85**, 056705 (2012)

Control-volume representation of molecular dynamics

E. R. Smith, D. M. Heyes, D. Dini, and T. A. Zaki*
Department of Mechanical Engineering, Imperial College London, Exhibition Road, London SW7 2AZ, United Kingdom
(Received 13 October 2011; revised manuscript received 2 March 2012; published 22 May 2012)

A molecular dynamics (MD) parallel to the control volume (CV) formulation of fluid mechanics is developed by integrating the formulas of Irving and Kirkwood [J. Chem. Phys. **18**, 817 (1950)] over a finite cubic volume of molecular dimensions. The Lagrangian molecular system is expressed in terms of an Eulerian CV, which yields an equivalent to Reynolds' transport theorem for the discrete system. This approach casts the dynamics of the molecular system into a form that can be readily compared to the continuum equations. The MD equations of motion are reinterpreted in terms of a Lagrangian-to-control-volume ($\mathcal{LCV}$) conversion function ϑ_i for each molecule i. The $\mathcal{LCV}$ function and its spatial derivatives are used to express fluxes and relevant forces across the control surfaces. The relationship between the local pressures computed using the volume average [Lutsko, J. Appl. Phys. **64**, 1152 (1988)] techniques and the method of planes [Todd *et al.*, Phys. Rev. E **52**, 1627 (1995)] emerges naturally from the treatment. Numerical experiments using the MD CV method are reported for equilibrium and nonequilibrium (start-up Couette flow) model liquids, which demonstrate the advantages of the formulation. The CV formulation of the MD is shown to be exactly conservative and is, therefore, ideally suited to obtain macroscopic properties from a discrete system.

DOI: 10.1103/PhysRevE.85.056705 PACS number(s): 05.20.−y, 47.11.Mn, 31.15.xv

Control Volume Function

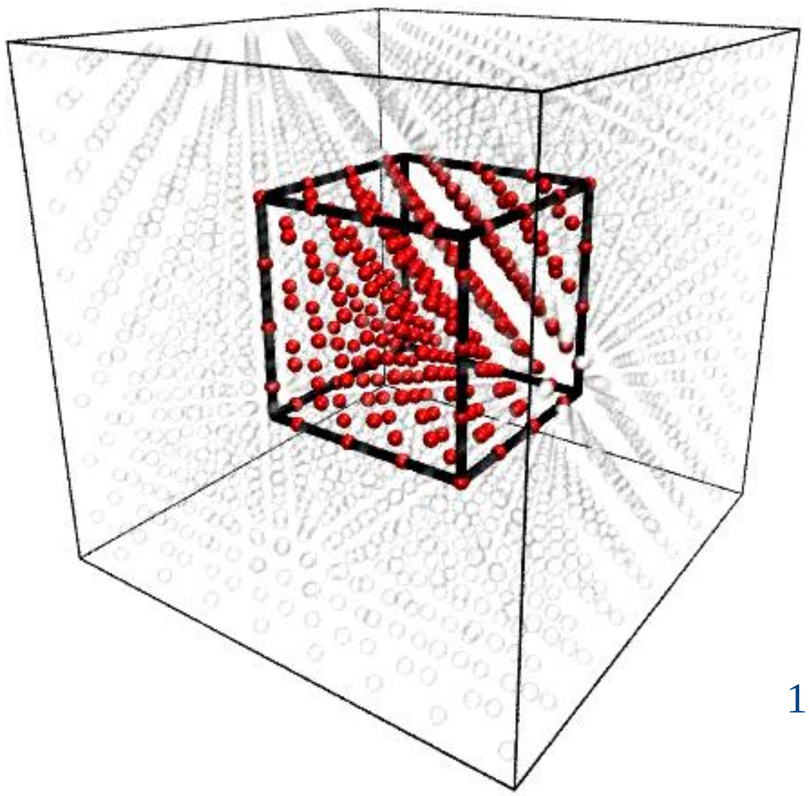
- **The Control Volume function is the integral of the Dirac delta function in 3 Dimensions**

$$\vartheta_i \equiv \int_{x^-}^{x^+} \int_{y^-}^{y^+} \int_{z^-}^{z^+} \delta(x_i - x)\delta(y_i - y)\delta(z_i - z)dxdydz$$

$$= \left[H(x^+ - x_i) - H(x^- - x_i)\right]$$

$$\times \left[H(y^+ - y_i) - H(y^- - y_i)\right]$$

$$\times \left[H(z^+ - z_i) - H(z^- - z_i)\right]$$



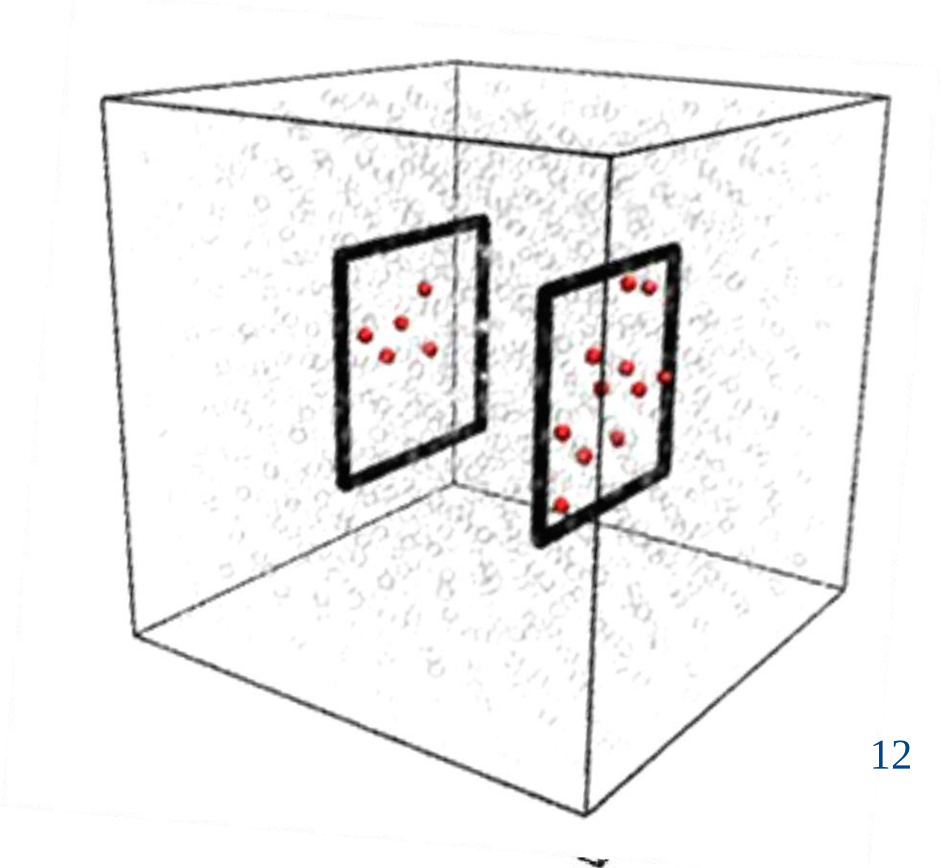
Derivatives yields the surface flux

- **Taking the Derivative of the CV function**

$$dS_{ix} \equiv -\frac{\partial \vartheta_i}{\partial x_i} = \left[\delta(x^+ - x_i) - \delta(x^- - x_i)\right]$$
$$\times \left[H(y^+ - y_i) - H(y^- - y_i)\right]$$
$$\times \left[H(z^+ - z_i) - H(z^- - z_i)\right]$$

- **Surface fluxes over the top and bottom surface**

$$dS_{ix} = dS_{ix}^+ - dS_{ix}^-$$



Applying the Control Volume Function

- **Molecular mass in a control volume can be defined**

$$\frac{d}{dt}\int_V \rho(\boldsymbol{r},t)\, dV = \frac{d}{dt}\sum_{i=1}^{N} m_i \vartheta_i(\boldsymbol{r}-\boldsymbol{r}_i)$$

- **Simple mathematical operations using the control volume function**

$$\frac{d}{dt}\sum_{i=1}^{N} m_i \vartheta_i = \sum_{i=1}^{N}\left(\vartheta_i \cancel{\frac{d}{dt}m_i} + m_i \frac{d}{dt}\vartheta_i\right)$$

$$= \sum_{i=1}^{N} m_i \frac{d\boldsymbol{r}_i}{dt}\cdot\frac{d}{d\boldsymbol{r}_i}\vartheta_i$$

$$= -\sum_{i=1}^{N} m_i \mathbf{v}_i \cdot d\mathbf{S}_i$$

Reynolds' Transport Theorem

- **Mass, momentum and energy equations**
  - Mass Conservation

$$\frac{d}{dt}\sum_{i=1}^{N} m_i\vartheta_i = -\sum_{i=1}^{N} m_i\mathbf{v}_i\cdot d\boldsymbol{S}_i \qquad \frac{\partial}{\partial t}\int_V \rho dV = -\oint_S \rho\boldsymbol{u}\cdot d\mathbf{S}$$

  - Momentum Balance

$$\frac{d}{dt}\sum_{i=1}^{N} m_i\mathbf{v}_i\vartheta_i = -\sum_{i=1}^{N} m_i\mathbf{v}_i\mathbf{v}_i\cdot d\mathbf{S}_i + \sum_{i=1}^{N}\sum_{j\neq i}^{N}\mathbf{f}_{ij}\vartheta_{ij}$$

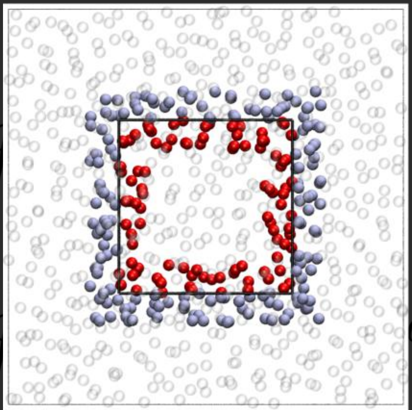
$$\frac{\partial}{\partial t}\int_V \rho\boldsymbol{u}dV = -\oint_S \rho\boldsymbol{u}\boldsymbol{u}\cdot d\mathbf{S} + \mathbf{F}_{\text{surface}}$$

- **The difference between two control volume functions for i and j**

$$\frac{d}{dt}\sum_{i=1}^{N} e_i\vartheta_i = -\sum_{i=1}^{N} e_i\mathbf{v}_i\cdot d\mathbf{S}_i + \frac{1}{2}\sum_{i=1}^{N}\sum_{i\neq j}^{N}\frac{\mathbf{p}_i}{m_i}\cdot \boldsymbol{f}_{ij}\vartheta_{ij}$$

$$\vartheta_{ij} \equiv \vartheta_i - \vartheta_j$$

$$\frac{\partial}{\partial t}\int_V \rho\mathcal{E}dV = - \ldots - \ldots d\mathbf{S}$$

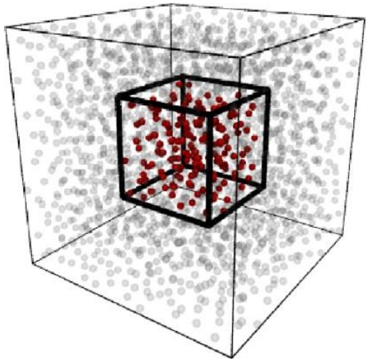


Testing Momentum Balance

- **Momentum Balance**

$$\underbrace{\frac{d}{dt}\sum_{i=1}^{N} m_i \dot{\mathbf{r}}_i \vartheta_i}_{\textit{Accumulation}} + \underbrace{\sum_{i=1}^{N} m \mathbf{v}_i \mathbf{v}_i \cdot d\mathbf{S}_i}_{\textit{Advection}} - \underbrace{\sum_{i=1}^{N} \sum_{j \neq i}^{N} \mathbf{f}_{ij} \vartheta_{ij}}_{\textit{Forcing}} = 0$$

$\frac{d}{dt}$



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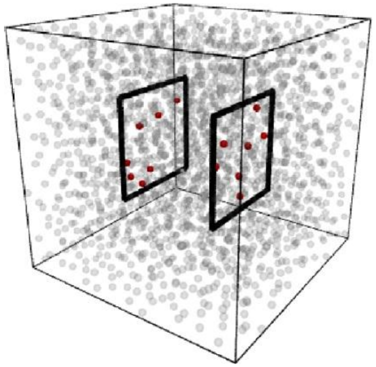

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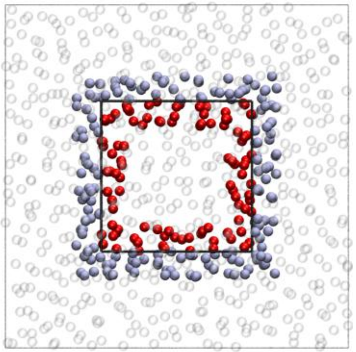
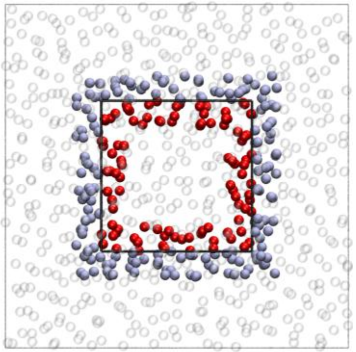


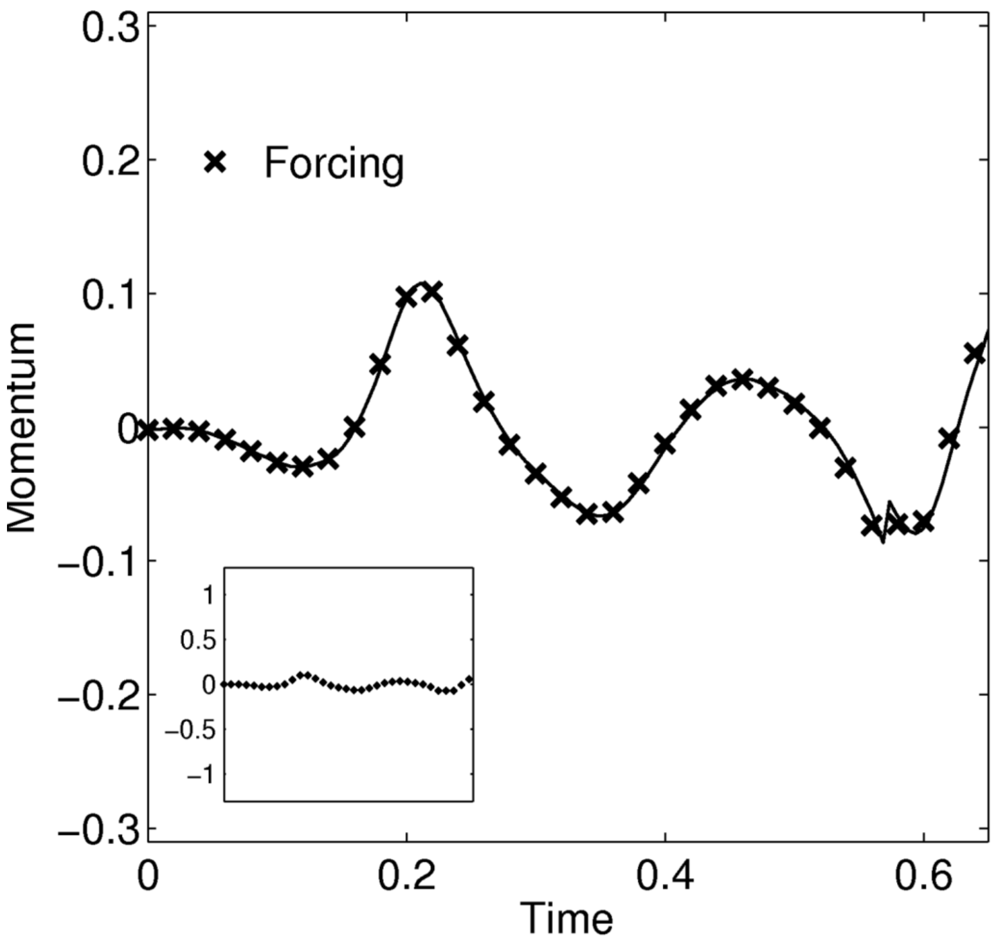
$= 0$

Testing Momentum Balance

- **Momentum Balance**

$$\underbrace{\sum_{i=1}^{N}\sum_{j\neq i}^{N}\mathbf{f}_{ij}\vartheta_{ij}}_{\textit{Forcing}}$$





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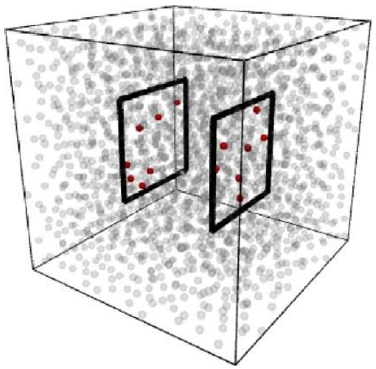
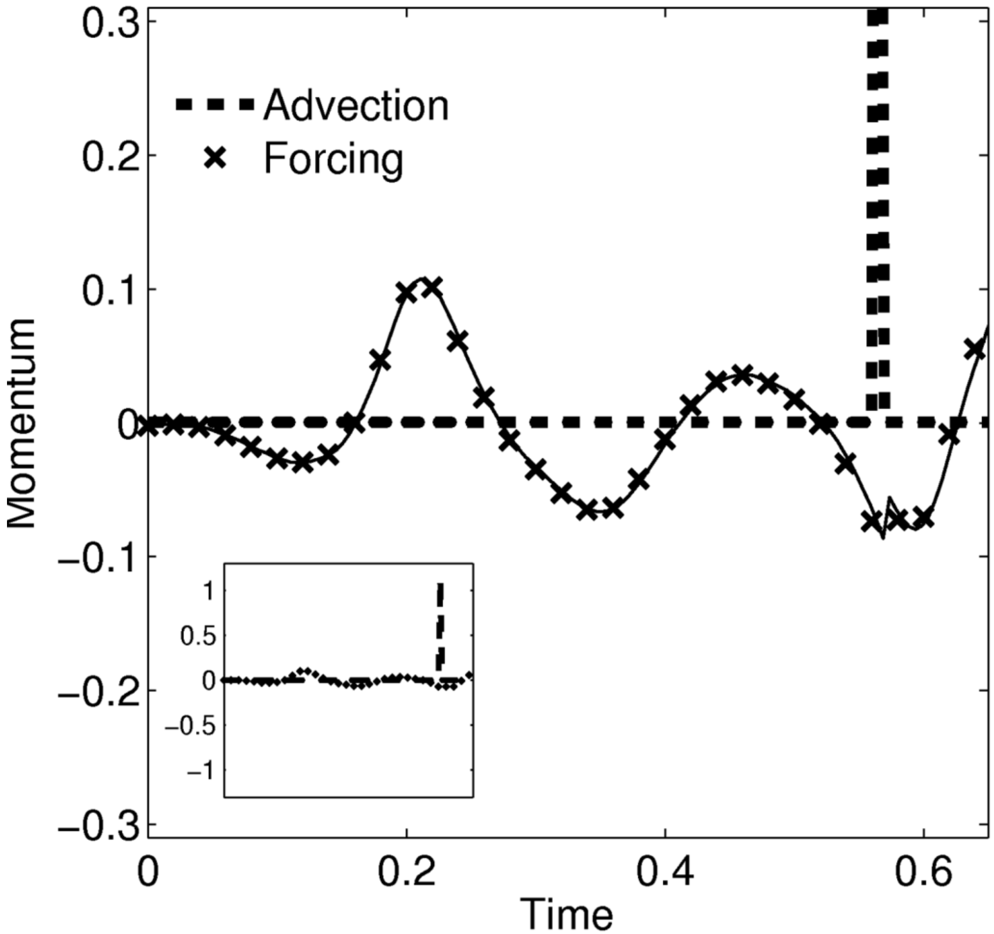
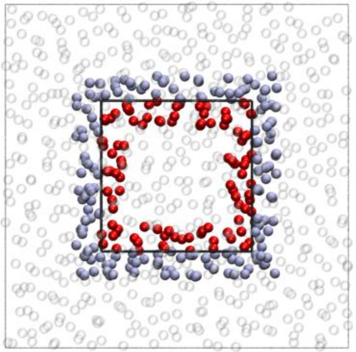
Testing Momentum Balance

- **Momentum Balance**

$$
\underbrace{-\sum_{i=1}^{N} m_i \mathbf{v}_i \mathbf{v}_i \cdot d\boldsymbol{S}_i}_{\textit{Advection}} + \underbrace{\sum_{i=1}^{N}\sum_{j\neq i}^{N} \mathbf{f}_{ij}\vartheta_{ij}}_{\textit{Forcing}}
$$







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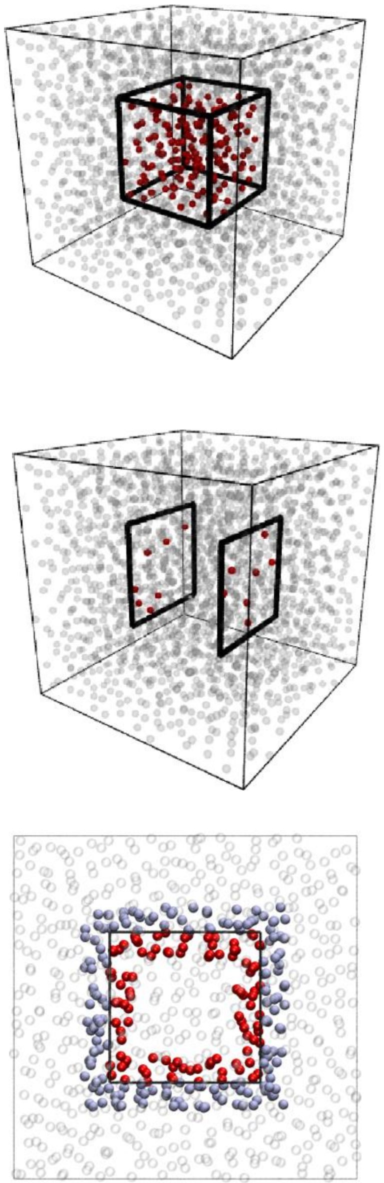
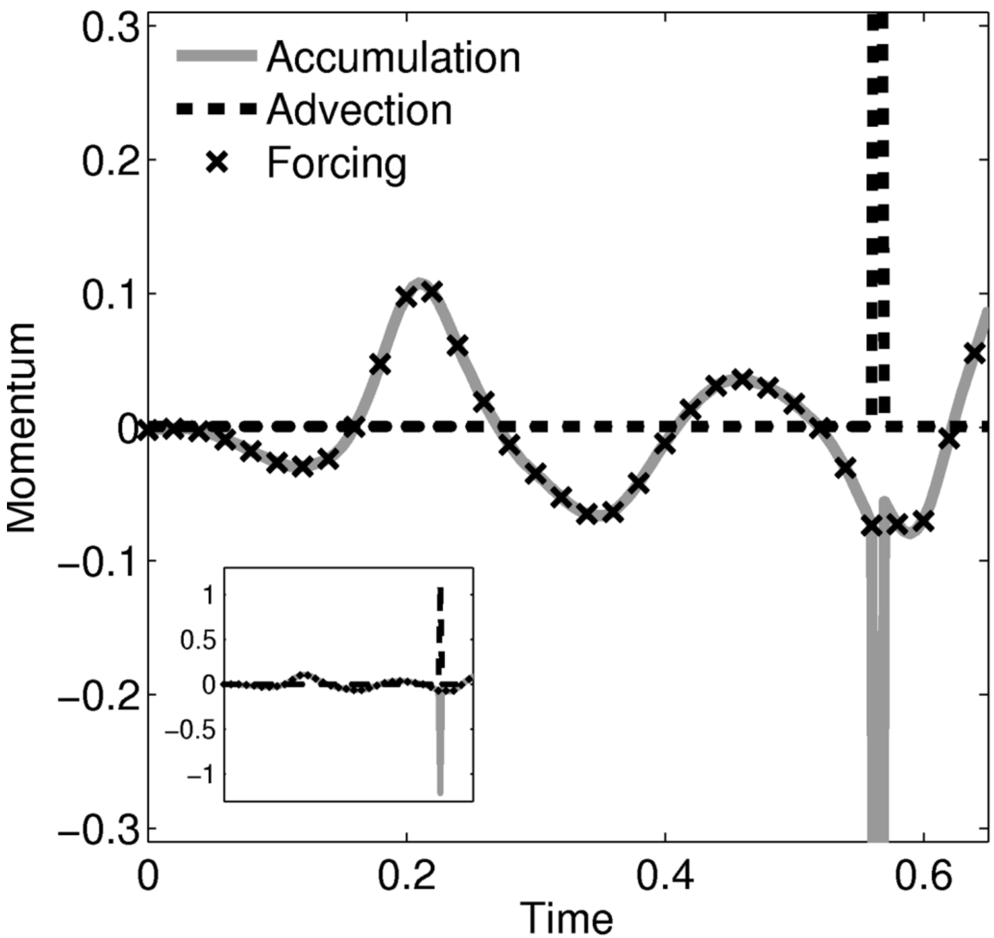
Testing Momentum Balance

- **Momentum Balance**

$$\underbrace{\frac{d}{dt}\sum_{i=1}^{N} m_i \mathbf{v}_i \vartheta_i}_{\textit{Accumulation}} = \underbrace{-\sum_{i=1}^{N} m_i \mathbf{v}_i \mathbf{v}_i \cdot d\boldsymbol{S}_i}_{\textit{Advection}} + \underbrace{\sum_{i=1}^{N}\sum_{j\neq i}^{N} \mathbf{f}_{ij}\vartheta_{ij}}_{\textit{Forcing}}$$

$$\frac{d}{dt}$$





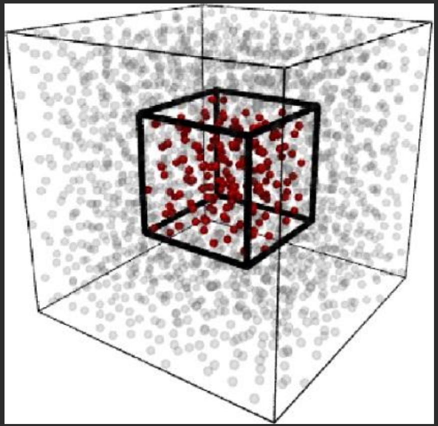
Divergence of Pressure

- **The momentum balance equation can be re-written in terms of the divergence of pressure**
  - Momentum Balance

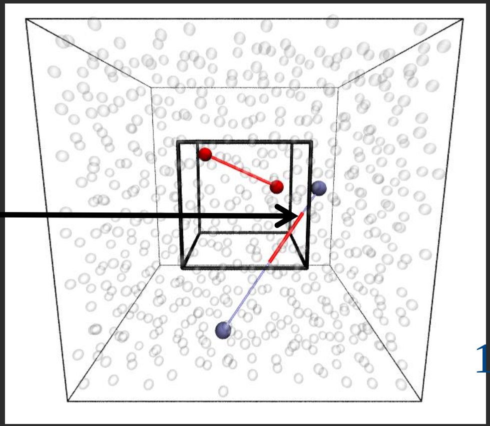
$$\frac{d}{dt}\sum_{i=1}^{N} m_i\mathbf{v}_i\vartheta_i = -\int_V \frac{\partial}{\partial \boldsymbol{r}}\cdot\rho\boldsymbol{u}\boldsymbol{u}d\mathbf{S}_i \qquad \frac{\partial}{\partial t}\int_V \rho\boldsymbol{u}dV = -\oint_S \frac{\partial}{\partial \boldsymbol{r}}\rho\boldsymbol{u}\boldsymbol{u}\cdot d\mathbf{S}$$

$$-\frac{\partial}{\partial \boldsymbol{r}}\cdot\sum_{i=1}^{N}\left[(\boldsymbol{v}_i - + \sum_{i=1}^{N}\sum_{j\neq i}^{N}\mathbf{f}_{ij}\vartheta_{ij} + \sum_{j\neq i}^{N}\boldsymbol{f}_{ij}\boldsymbol{r}_{ij}\int_0^1 \vartheta_s ds\right] \qquad -+\mathbf{F}_{\mathrm{surface}}\int_V\frac{\partial}{\partial \boldsymbol{r}}\mathbf{\Pi}dV$$

- **Volume Average Form of Lutsko (1988) & Cormier et al (2001)**



$$\vartheta_{ij} = \sum_{\alpha=1}^{3}\frac{\partial}{\partial r_\alpha}\boxed{\int_0^1 \vartheta_s ds}$$



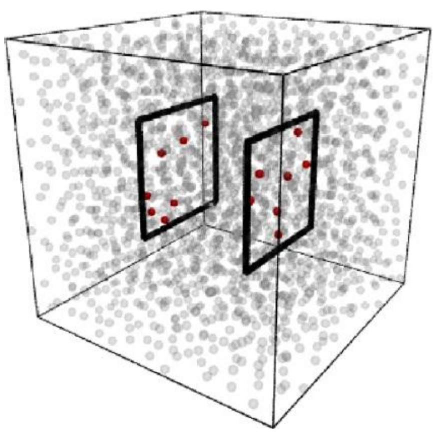
Surface Pressures

- **The momentum balance equation can be re-written in terms of pressure over the control volume surfaces**
  - Momentum Balance

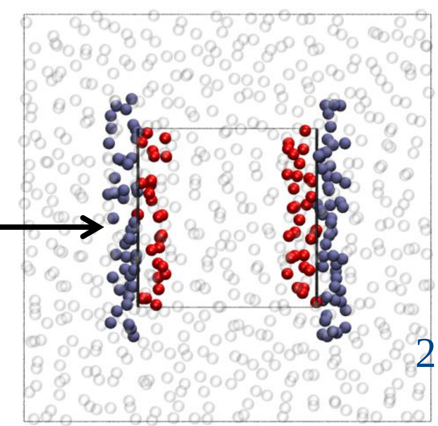
$$\frac{d}{dt}\sum_{i=1}^{N} m_i \mathbf{v}_i \vartheta_i = -\oint_S \rho \boldsymbol{u}\boldsymbol{u} \cdot d\boldsymbol{S} \qquad \frac{\partial}{\partial t}\int_V \rho \boldsymbol{u} dV = -\oint_S \rho \boldsymbol{u}\boldsymbol{u} \cdot d\boldsymbol{S}$$

$$-\frac{\partial}{\partial \boldsymbol{r}} \cdot \sum_{i=1}^{N}\sum_{i=1}^{N}\left[(\boldsymbol{v_i} - \boldsymbol{u})(\boldsymbol{v_i} - \boldsymbol{u}) \vartheta_i d\boldsymbol{S}_i \sum_{j \neq i}^{N} \sum_{i=1}^{N} \boldsymbol{f}_{ij} \boldsymbol{r}_{ij} \sum_{j \neq i}^{N} \int_0^1 \boldsymbol{f}_{ij} \vartheta_s ds \, d\boldsymbol{S}_{ij} \right] \qquad -\int_V \oint_S \frac{\partial}{\partial \boldsymbol{r}} \boldsymbol{\Pi} \cdot d\boldsymbol{S} dV$$

- **The derivative of ϑ_s is the forces acting over the surface a localisation of the method of planes (Todd et al 1995)**



$$\vartheta_{ij} = \sum_{\alpha=1}^{3} \frac{\partial}{\partial r_\alpha} \int_0^1 \vartheta_s ds = dS_{xij} + dS_{yij} + \boxed{dS_{zij}} \rightarrow$$



Results and Applications

Unsteady Couette Flow

- **Continuum Analytical**
  - Simplify the momentum balance (Navier-Stokes) equation

$$\frac{\partial}{\partial t}\boldsymbol{u} + \boldsymbol{\nabla}\cdot\cancel{\boldsymbol{u}\boldsymbol{u}} = \frac{1}{\rho}\cancel{\boldsymbol{\nabla}P} + \frac{\mu}{\rho}\boldsymbol{\nabla}^2\boldsymbol{u}$$

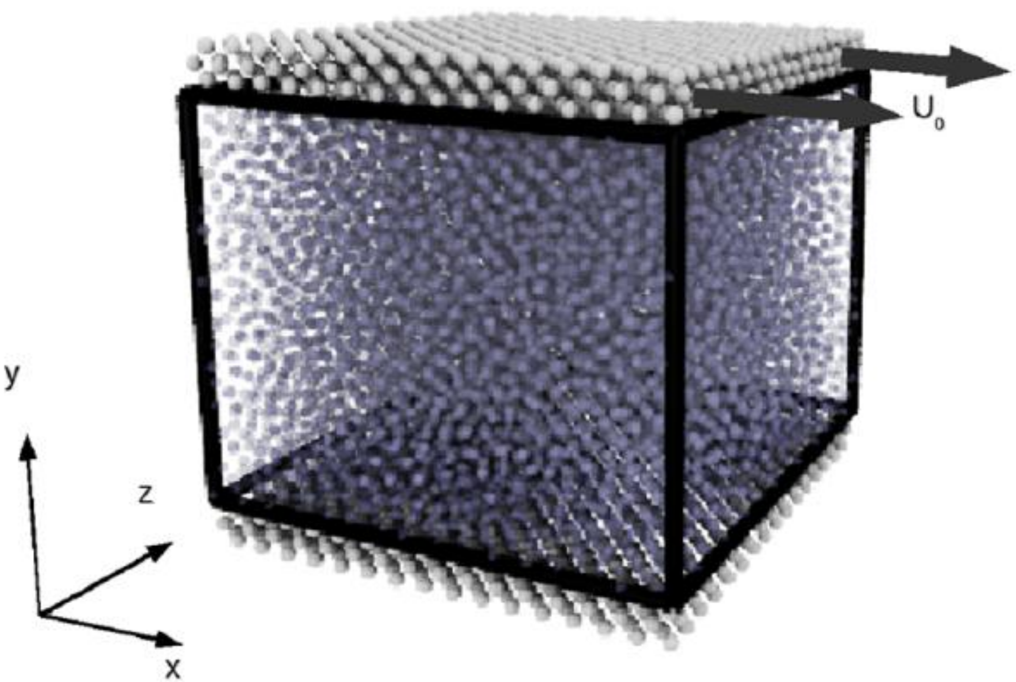
  - Solve the 1D unsteady diffusion equation.

$$\frac{\partial u_x}{\partial t} = \frac{\mu}{\rho}\frac{\partial^2 u_x}{\partial y^2}$$

  - With Boundary Conditions

$$u_x(0,t) = 0$$
$$u_x(L,t) = U_0$$
$$u_x(y,0) = 0$$

- **Molecular Dynamics**
  - Fixed bottom wall, sliding top wall with both thermostatted



Unsteady Couette Flow

- **Continuum Analytical**
  - Simplify the control volume momentum balance equation

$$\frac{\partial}{\partial t}\int_V \rho \boldsymbol{u} dV = -\oint_S \cancel{\rho \boldsymbol{u}\boldsymbol{u}} \cdot d\boldsymbol{S} - \oint_S \cancel{P\boldsymbol{I}} \cdot d\boldsymbol{S} + \oint_S \boldsymbol{\sigma} \cdot d\boldsymbol{S}$$

  - Simplifies for a single control volume

$$\frac{\partial}{\partial t}\int_V \rho u_x dV = \int_{S_y^+} \sigma_{xy} dS_f^+ - \int_{S_f^-} \sigma_{xy} dS_y^-$$

  - With Boundary Conditions

$$u_x(0,t) = 0$$
$$u_x(L,t) = U_0$$
$$u_x(y,0) = 0$$

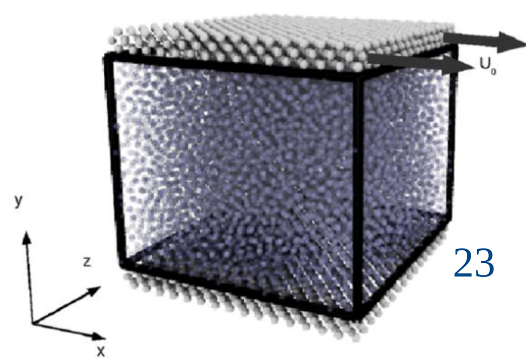
- **Molecular Dynamics**
  - Discrete form of the Momentum balance equation

$$\frac{d}{dt}\sum_{i=1}^{N} m_i \mathbf{v}_i \vartheta_i = -\oint_S \cancel{\rho \boldsymbol{u}\boldsymbol{u}} \cdot d\boldsymbol{S} - \sum_{i=1}^{N} \cancel{(\boldsymbol{v}_i - \boldsymbol{u})(\boldsymbol{v}_i - \boldsymbol{u})} \cdot d\boldsymbol{S}_i - \sum_{i=1}^{N}\sum_{j\neq i}^{N} \varsigma_{ij} \cdot d\boldsymbol{S}_{ij}$$

  - Simplifies for a single control volume

$$\frac{d}{dt}\sum_{i=1}^{N} m_i \mathbf{v}_i \vartheta_i = \sum_{i,j}^{N} f_{xij} dS_{yij}^+ - \sum_{i,j}^{N} f_{xij} dS_{yij}^-$$

  - Fixed bottom wall, sliding top wall with both thermostatted

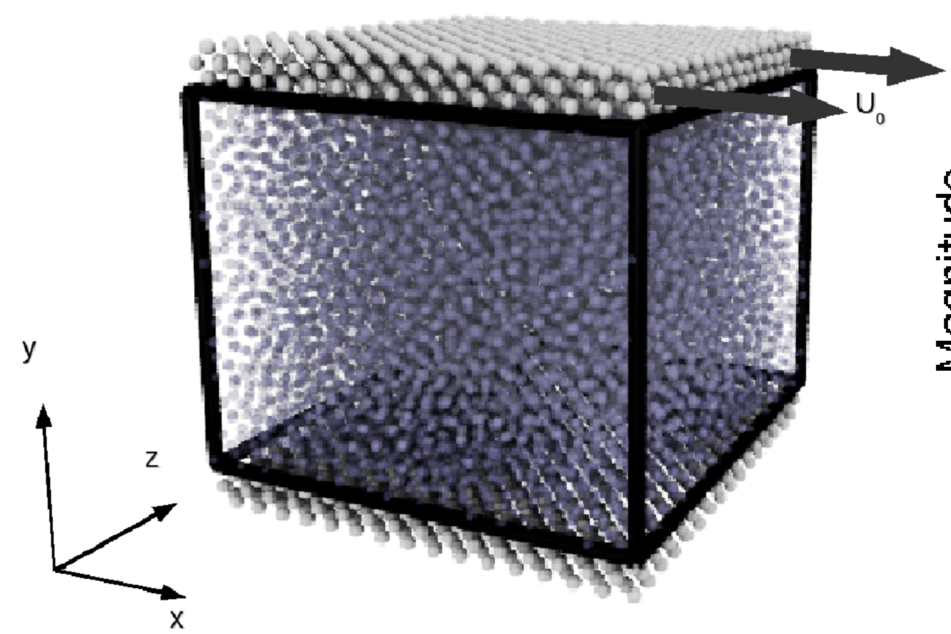


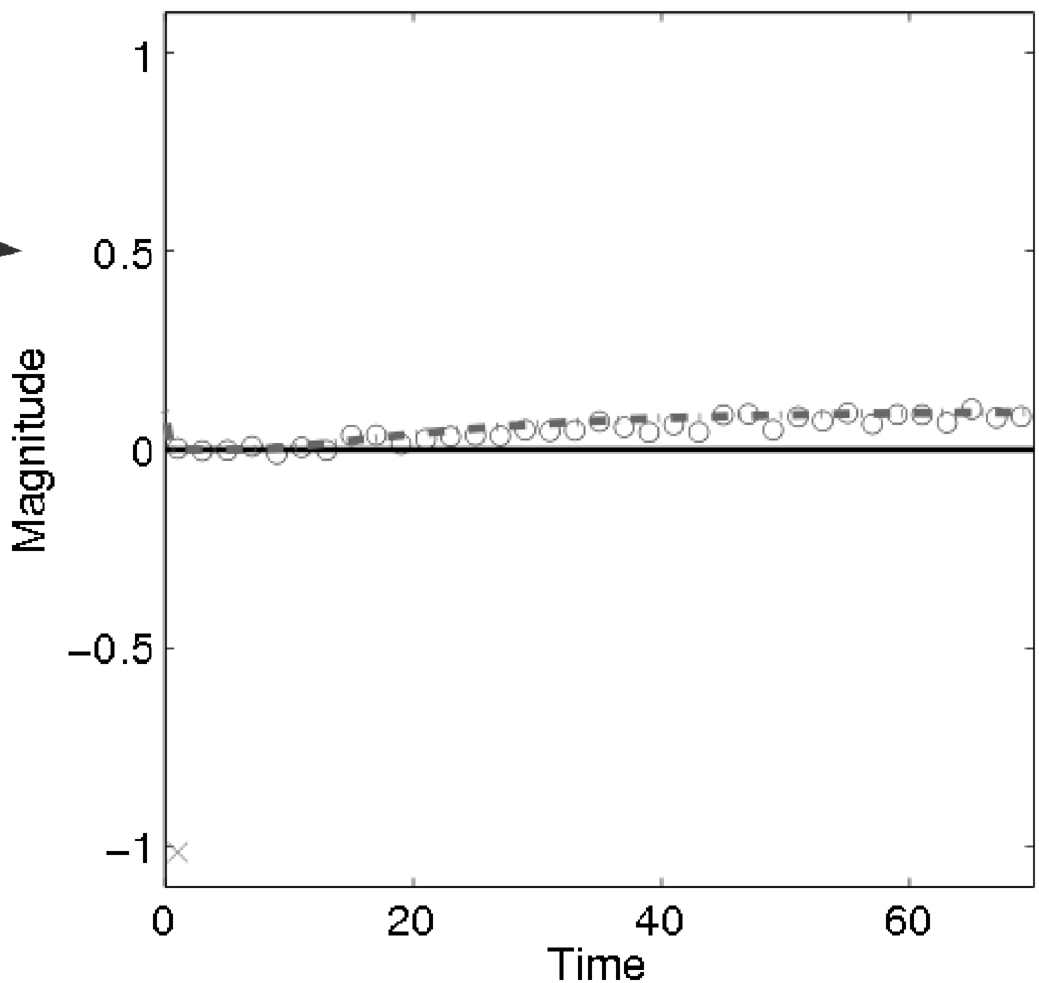
Unsteady Couette Flow

- **Simulation setup**
  - Starting Couette flow
  - Wall thermostat: Nosé-Hoover
  - Averages are computed over 1000 time steps and 8 realizations

$$\frac{d}{dt}\sum_{i=1}^{N} m_i \mathbf{v}_i \vartheta_i = \sum_{i,j}^{N} f_{xij} dS_{yij}^{+} - \sum_{i,j}^{N} f_{xij} dS_{yij}^{-}$$

$$\frac{\partial}{\partial t}\int_V \rho u_x dV = \int_{S_f^+} \Pi_{xy} dS_f^{+} - \int_{S_f^-} \Pi_{xy} dS_f^{-} .$$





Unsteady Couette Flow

- **Simulation setup**
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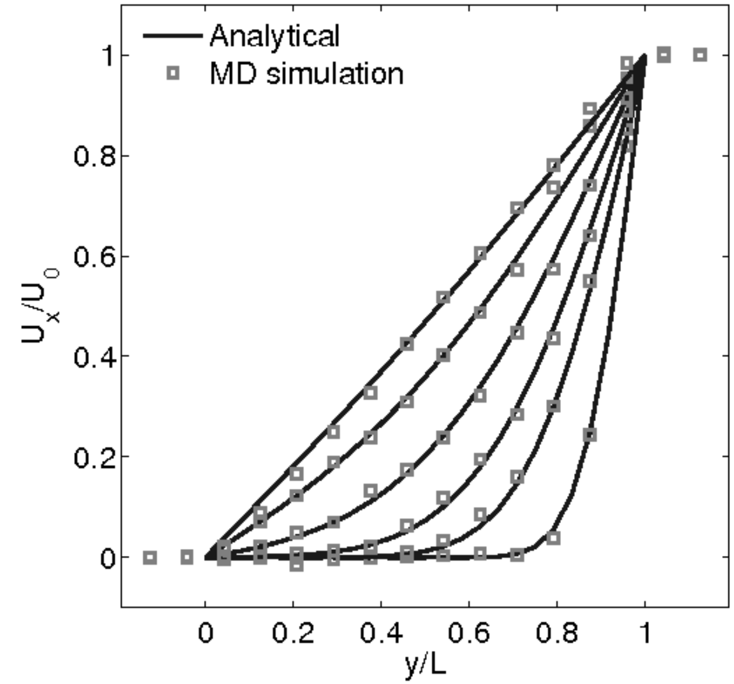
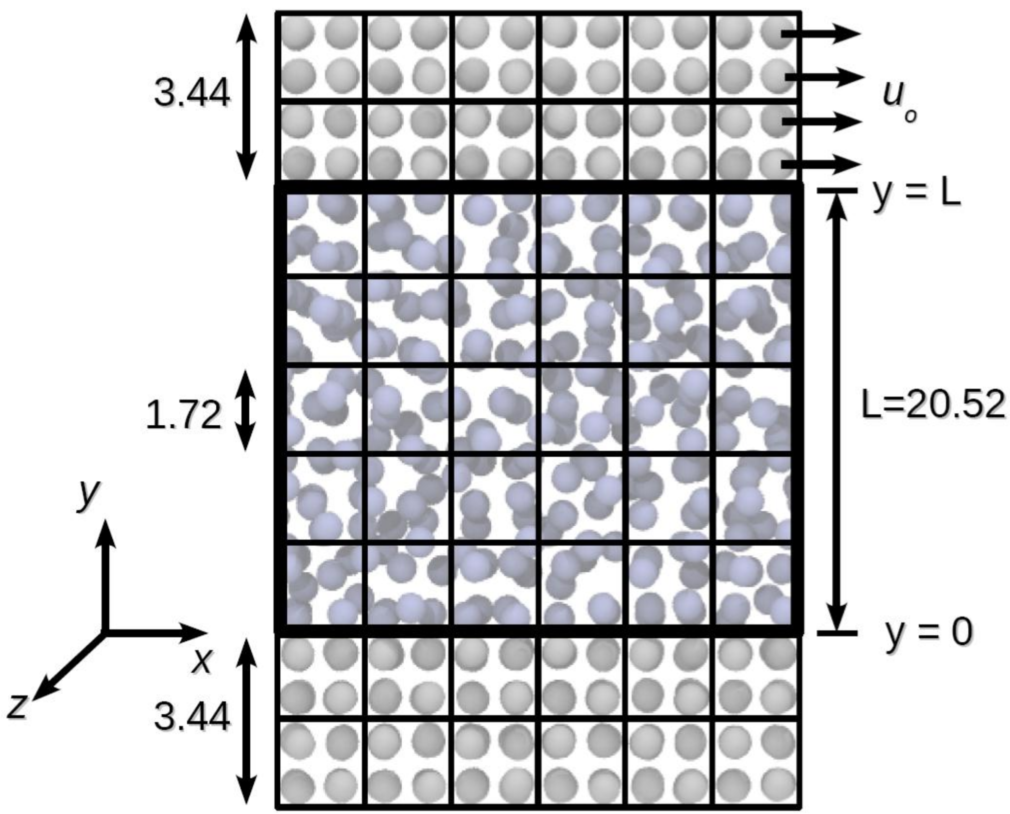
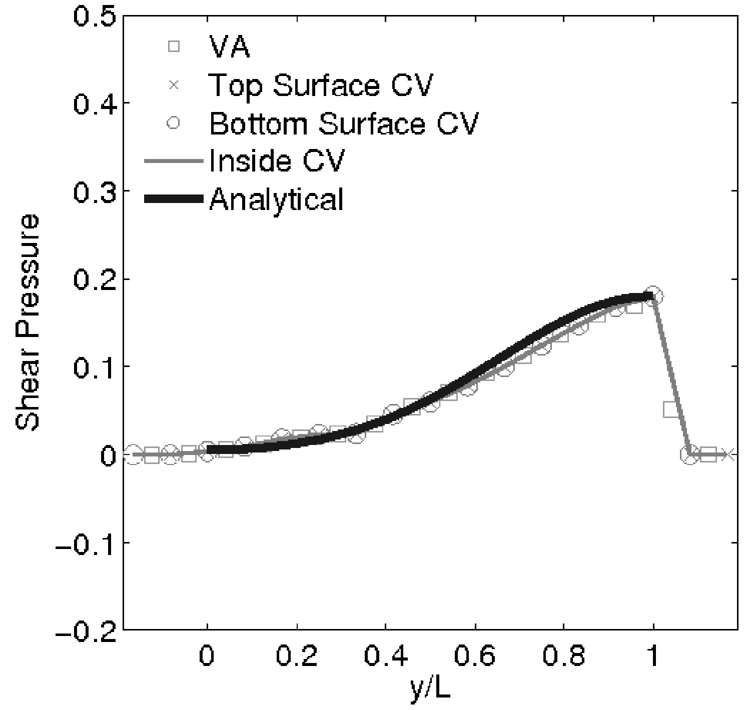




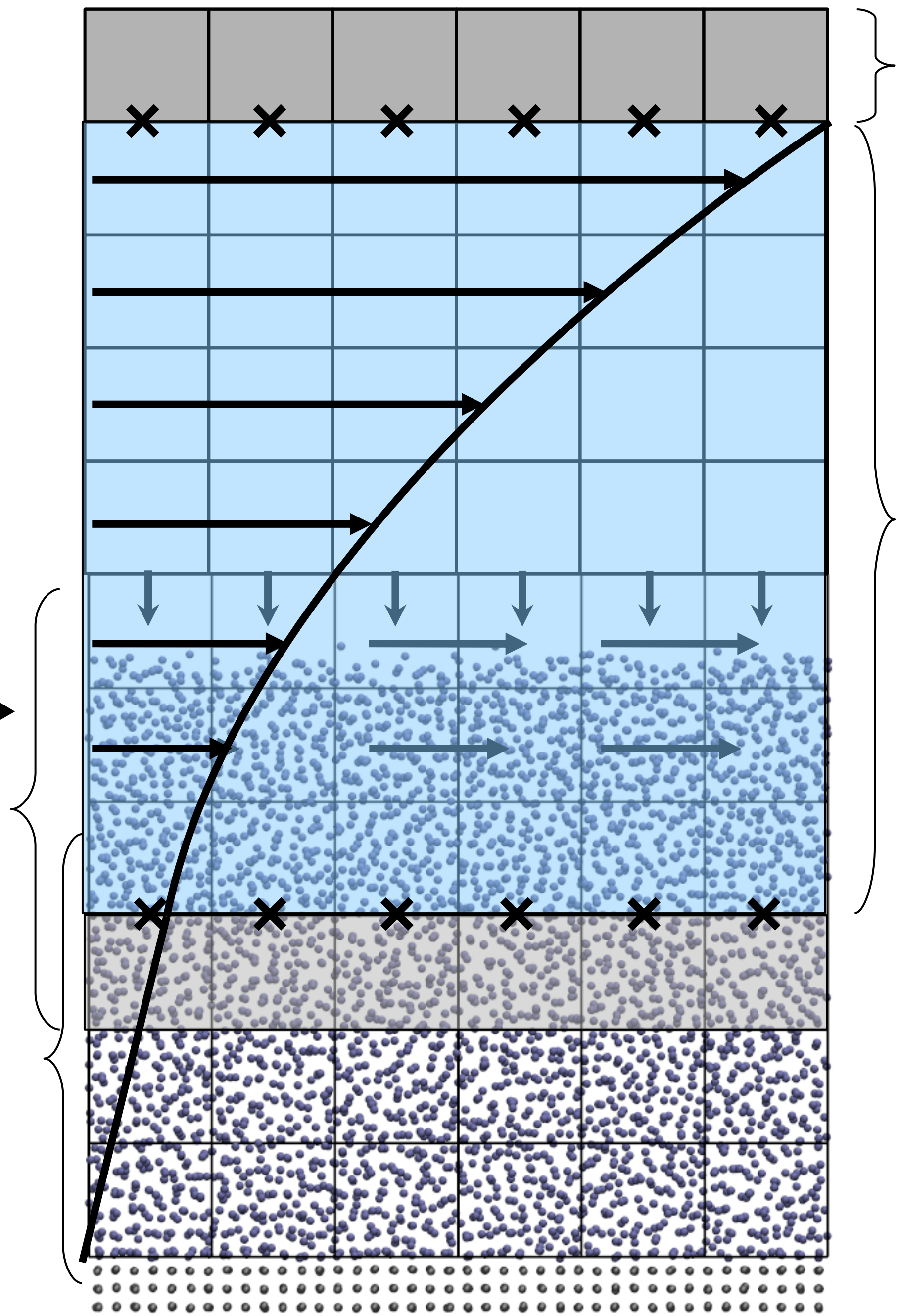


Coupling

- **Molecular Equations**

$$\frac{d}{dt}\sum_{i=1}^{N} m_i \mathbf{v}_i \vartheta_i = -\oint_S \rho \boldsymbol{u}\boldsymbol{u}\cdot d\boldsymbol{S} - \sum_{i=1}^{N} \left(\boldsymbol{v}_i - \boldsymbol{u}\right)\left(\boldsymbol{v}_i - \boldsymbol{u}\right)\cdot d\boldsymbol{S}_i - \sum_{i=1}^{N}\sum_{j\neq i}^{N} \varsigma_{ij}\cdot d\boldsymbol{S}_{ij}$$

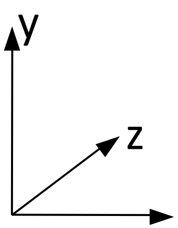
$$m\ddot{\mathbf{r}}_i = \sum_{j\neq i}^{N} \mathbf{f}_{ij}$$



$$\rho u = \rho U_0$$

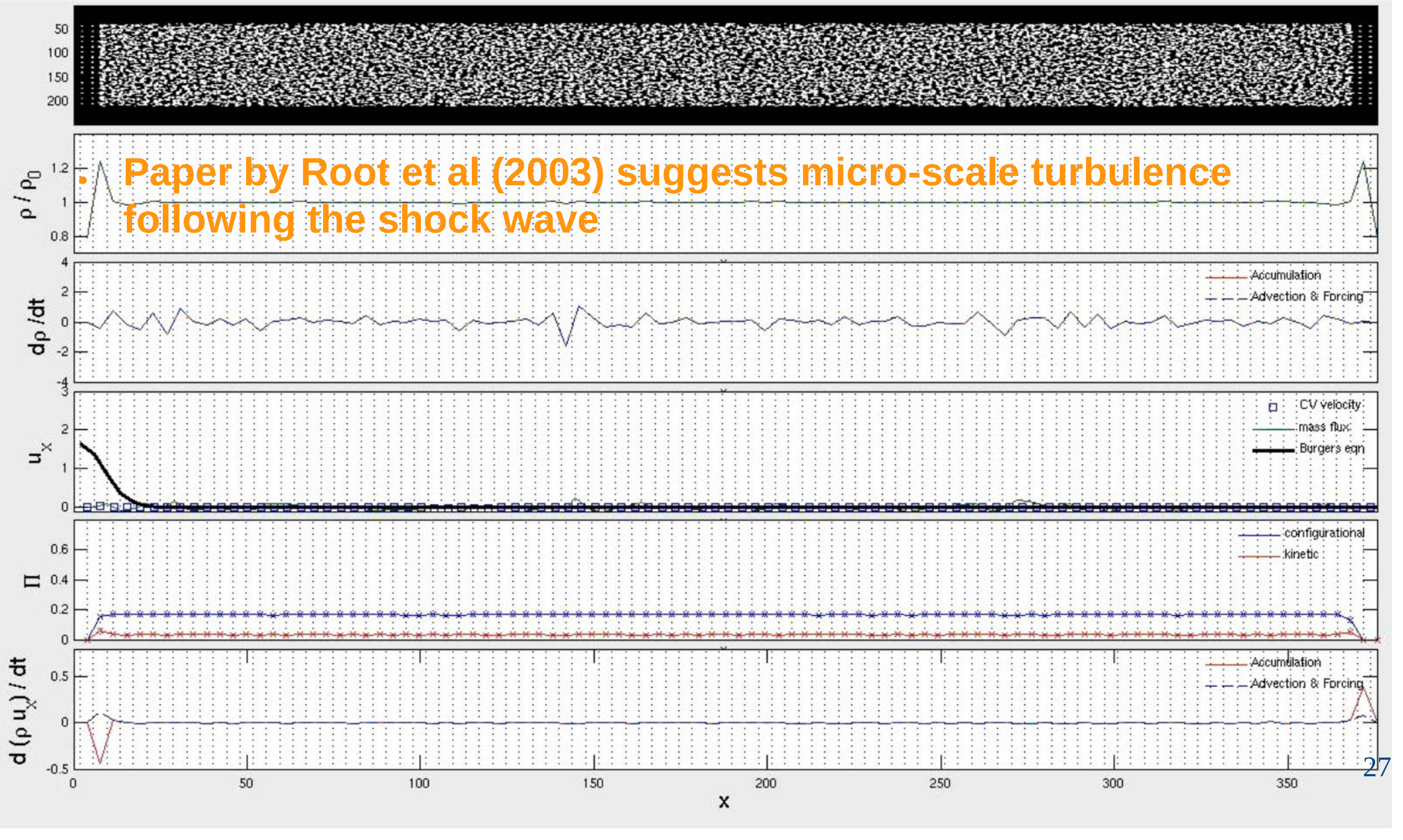
$$\frac{\partial}{\partial t}\int_V \rho \boldsymbol{u} dV = -\oint_S \rho \boldsymbol{u}\boldsymbol{u}\cdot d\boldsymbol{S} - \oint_S \boldsymbol{\Pi}\cdot d\boldsymbol{S}$$

- **Continuum Equations**



Shockwaves

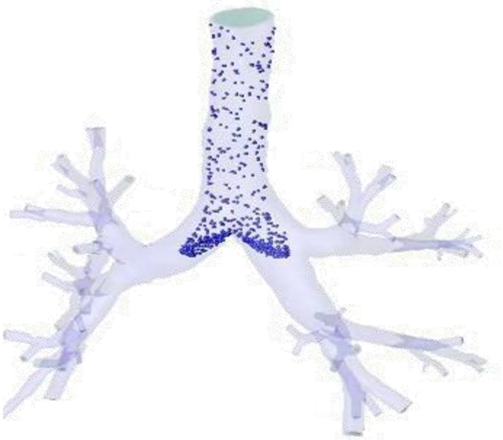
- Current work on application of control volume theory



- Paper by Root et al (2003) suggests micro-scale turbulence following the shock wave

Other Possible Applications

- **Particles laden continuum flows**
  - Sediment transfer in rivers
  - Tracer particles in flow analysis
- **Vortex particle methods**
  - Discrete Lagrangian vortices which interact
- **Other discrete meso-scale methods**
  - Brownian dynamics
  - Dissipative particle dynamics
  - Smooth particle hydrodynamics
- **Analysis of results from discrete experiments**
  - Volumetric 3-component velocimetry



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Summary

- **Introduced a novel mathematical function to defines a control volume in a discrete system**
  - Derived in a manner consistent with a continuum form of the control volume
  - Mathematically well defined and applicable to any discrete system
- **Reynolds' transport theorem is extended beyond the continuum**
  - Allows control volume analysis to be extended to nano-scale systems
  - The resulting equations are exactly conservative in a discrete system
- **The resulting formulation has a number of applications**
  - Give a consistent and intuitive form of molecular pressure – showing the connection between two widely used descriptions in the literature
  - Semi-analytical solution to problems like Couette flow
  - Facilitates a rigorous derivation of coupling strategies
  - Analysis of shockwaves and insight into molecular level turbulence.

References/Acknowledgments

- **Acknowledgments**
  - My supervisors; Professor D.M. Heyes, Dr D. Dini and Dr T.A. Zaki
  - Dr Nolan for his photographs
- **References**

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- **Thank you for listening**
- **Any Questions?**

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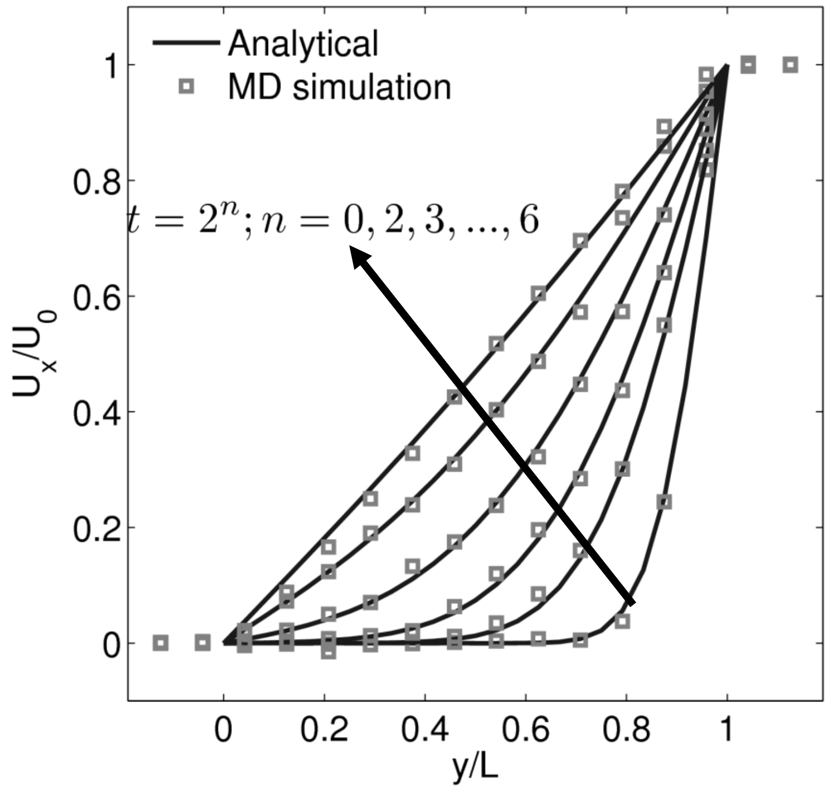
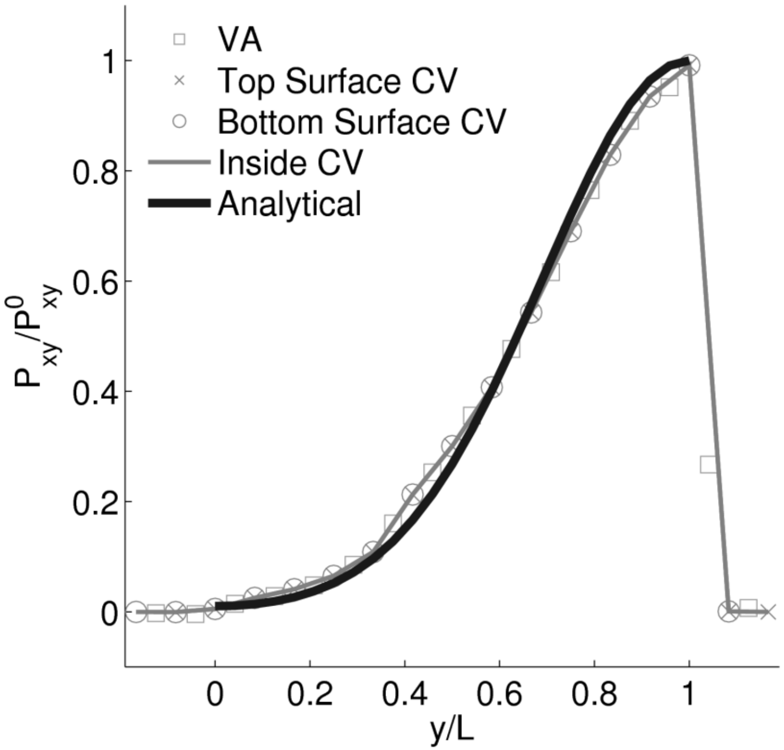
Continuum Analytical Couette Flow





$$u_x(y,t) = \begin{cases} U_0 & y = L \\ \sum_{n=1}^{\infty} u_n(t) sin\left(\frac{n\pi y}{L}\right) & 0 < y < L \\ 0 & y = 0 \end{cases}$$

$$\Pi_{xy}(y,t) = \frac{\mu U_0}{L}\left[1 + 2\sum_{n=1}^{\infty}(-1)^n e^{-\frac{\lambda_n \mu t}{\rho}} cos\left(\frac{n\pi y}{L}\right)\right]$$

$$\text{Where, } \lambda_n = \left(\frac{n\pi}{L}\right)^2 \text{ and } u_n(t) = \frac{2U_0(-1)^n}{n\pi}\left(e^{-\frac{\lambda_n \mu t}{\rho}} - 1\right)$$

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Moving reference frame

- **Why the continuum form of Reynolds' transport theorem has a partial derivative but the discrete is a full derivative**
  - Eulerian mass conservation

$$\vartheta_i = \vartheta_i(\boldsymbol{r}_i(t), \boldsymbol{r})$$

$$\frac{d}{dt}\sum_{i=1}^{N} m_i \vartheta_i = -\sum_{i=1}^{N} m_i \mathbf{v}_i \cdot d\boldsymbol{S}_i$$

$$\frac{\partial}{\partial t}\int_V \rho dV = -\oint_S \rho \boldsymbol{u} \cdot d\mathbf{S}$$

  - Lagrangian mass conservation

$$\vartheta_i = \vartheta_i(\boldsymbol{r}_i(t), \boldsymbol{r}(t))$$

$$\frac{d}{dt}\sum_{i=1}^{N} m_i \vartheta_i = -\sum_{i=1}^{N} m_i \left(\mathbf{v}_i + \overline{\boldsymbol{u}}\right) \cdot d\boldsymbol{S}_i$$

$$\frac{d}{dt}\int_V \rho dV = \oint_S \rho \left(\boldsymbol{u} - \overline{\boldsymbol{u}}\right) \cdot d\boldsymbol{S}$$

$$\overline{\boldsymbol{u}} \cdot d\boldsymbol{S}_i = \frac{d\boldsymbol{r}}{dt} \cdot \frac{d\vartheta_i}{d\boldsymbol{r}}$$

$$\oint_S \rho \boldsymbol{u} \cdot d\boldsymbol{S} - \oint_S \rho \overline{\boldsymbol{u}} \cdot d\boldsymbol{S} = 0$$